Chapter 2

Review of Diffusion Models

In this chapter, mathematical models used to describe compressible fluid flow through porous media, are reviewed. The diffusion equation governing the flow can be derived by performing a mass balance on the fluid within a control volume. Thereby, an insight, into diffusion models, gives the fundamental knowledge of the process and some modeling related issues for fluid flow.

2.1 Mathematical Modeling

Modeling is a process of describing the system using mathematical concepts and language. The mathematical modeling cycle begins with a situation in the real world, as shown in Figure 2.1. The close study of the system, the accumulation and organization of information, is really the first step in model building.
An important aspect of modeling cycle is to identify and to select those concepts to be considered as basic in the study and to define them carefully. This cycle typically involves making certain idealizations and approximations. The purpose here is to eliminate unnecessary information and to simplify that which is retained as much as possible.

The expression of the entire practical operation in symbolic terms, is major part of modeling. As a consequence, the real world problem becomes a mathematical model in which the real quantities and processes are replaced by mathematical symbols and relations (sets, functions, equations, etc.) and mathematical operations.

After the problem has been transformed into symbolic terms, the resulting mathematical system is studied using appropriate mathematical ideas and techniques. The results of the mathematical study are theorems from a mathematical point of view and predictions, from the empirical point of view.

The final step in the model-building process is the comparison of the results predicted on the basis of the mathematical work with the real world.

Hence in the nutshell, the process of modeling involves the knowledge of the system, essential features of the process, formulation of model, solution of the model, interpretation of the results and the comparison with the experimental and observational values, if possible.

Simulation and modeling are two essential blocks of modeling for industrial problems. The motivation behind mathematical modeling is to gain understanding of physical phenomenon and to predict the actual process. Normally, partial differential equations
(PDEs) arise in the mathematical description of a spectrum of chemical and physical problems. Simulation enables inquiry into the possibility of implementation of the model and limitations of the model.

2.2 Mass Transfer and Mass Exchange Theory during Washing Process

The analysis of system of industrial problems like pulp washing needs constantly growing use of modeling. The mass transfer rates between the bulk fluid phase and particle phase are dominated by three phenomena: convection, diffusion and dispersion. The mass transfer due to convection and dispersion occurs in bulk fluid phase. The mass exchange between the bulk fluid and particle phase takes place by diffusion through the film of solvent surrounding the particle. In principle, adsorptive exchange takes place all over the particle surface. However, for case of modeling, only the pore phase is supposed to be in exchange with the particle surface, and the exchange between the particle phase and the bulk fluid phase through the film. This mechanism is illustrated in Figure 2.2.

From fluid dynamics and mass transfer, mathematical descriptions are available for the above three phenomena. The level of mathematical difficulty encountered, depends much on the nature of equilibrium, relationship, the concentration level, and choice of flow mode. According to Ruthven [84], model complexity should be analyzed from the following classification:
• Nature of equilibrium relationship (linear isotherm or nonlinear isotherm)

• Isothermal (heat transfer resistance can be neglected)

• Concentration level of mixed components (components with low or high concentration)

• Flow pattern (plug flow or dispersed plug flow)

• Complexity of kinetic model

  1. Negligible mass transfer resistance

  2. Single mass transfer resistance (either external film control or intraparticle diffusion control)

  3. Two mass transfer resistance (external film along with interparticle diffusion or macropore-micropore internal diffusion resistance)

  4. Three mass transfer resistance (external film along with two internal diffusion)

Based on the mass transfer and mass exchange theory during washing process, in the following section, the models are summarised available from literature in a systematic way to help the understanding of their suitability.

### 2.3 Review of Existing Diffusion Models

The ways of describing mass transfer resistance between the bulk fluid phase and porous particle phase make a big contribution in the complexity of the models.
It may be treated either according to equilibrium theory or by including an appropriate rate expression to account for the mass transfer resistance, generally in terms of diffusion models. All equilibrium models use isotherm equation directly to represent the relationship between the concentration on particle surface and in bulk fluid phase. While, diffusion models are the application of the first Fick’s law of mass transport and are the equations of equilibrium isotherm.

Although, various models have been developed time to time by the investigators to explain the washing behavior during flow through packed bed of solid particles. A brief description of models proposed by previous researchers along with their respective initial and boundary conditions is presented hereunder.

Kuo [53] has studied washing of filter cakes by assuming that mass transfer exists between the stagnant film and the bulk fluid. The flow channel and the filtrate film were taken to be uniform cross section with transport of solute between the wash liquor and the filtrate occurring at the rate proportional to the solute concentration. The model equations were solved analytically by using Laplace transforms.

Wash liquor model

$$\frac{\partial C}{\partial T} = k_1(N - C) - U \frac{\partial C}{\partial X}. \quad (2.1)$$

Stagnant film model

$$\frac{\partial N}{\partial T} = k_2(C - N). \quad (2.2)$$

Initial condition

$$C = C_0 \text{ and } N = N_0, \quad \text{ at } T = 0. \quad (2.3)$$
Brenner [18] has presented an axial dispersion model ignoring the concentration of the solute adsorbed on particle surface and the porosity of the packed bed. He gave the basic model for washing zone considering Danckwert’s boundary conditions.

Axial dispersion model

\[
\frac{\partial C}{\partial T} = D_L \frac{\partial^2 C}{\partial X^2} - U \frac{\partial C}{\partial X}. \tag{2.4}
\]

Boundary conditions

\[
UC - D_L \frac{\partial C}{\partial X} = UC_s, \quad \text{at } X = 0, \tag{2.5}
\]

\[
\frac{\partial C}{\partial X} = 0, \quad \text{at } X = L. \tag{2.6}
\]

Initial condition

\[
C = C_0, \quad \text{at } T = 0. \tag{2.7}
\]

The model has its application in both the solid and semi solid particles having spherical or cylindrical particle geometry. The model was solved using Laplace transforms. Brenner [18] has presented the numeric values of exit and average solute concentrations at different times for different values of Peclet number ranging between 0 to \( \infty \).

Sherman [91] has considered concentration of solute adsorbed on particle surface and porosity of the bed. Step input boundary conditions were followed.

Axial dispersion model

\[
\frac{\partial C}{\partial T} + \left( \frac{1 - \epsilon}{\epsilon} \right) \frac{\partial N}{\partial T} = D_L \frac{\partial^2 C}{\partial X^2} - U \frac{\partial C}{\partial X}. \tag{2.8}
\]
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Boundary condition

\[ C = C_0(k_0 + k_1T + k_2T^2 + k_3T^3 + k_4T^4)e^{-\gamma T}, \quad \text{at } X = 0. \] (2.9)

Initial condition

\[ C = C_0, \quad \text{at } T = 0, \] (2.10)

where \( \gamma \) is constant and \( k_0, k_1, k_2, k_3, k_4 \) were so adjusted that the analytic values agree with the experimental values via experimentally determined curve of \( C \) versus \( T \). The bulk fluid concentration and the concentration of solute adsorbed on the fiber surface were related via linear adsorption isotherm. The model was solved using Laplace transforms.

Pellett [73] has developed an extended model for washing of synthetic fibers and glass beads. The effects of both axial dispersion and intrafiber diffusion were combined by dividing bed into zones of external fluid and particle diffusion.

Axial dispersion model

\[ \frac{\partial C}{\partial T} + \left(1 - \frac{\epsilon}{\epsilon} \right) \frac{\partial Q}{\partial T} = D_L \frac{\partial^2 C}{\partial X^2} - U \frac{\partial C}{\partial X}. \] (2.11)

Particle phase model

\[ D_F \left(\frac{\partial^2 Q}{\partial r^2} + \frac{\nu}{r} \frac{\partial Q}{\partial r}\right) = \frac{\partial Q}{\partial T}. \] (2.12)

\( \nu \) stands for particle geometry and takes value 1, 2 or 3 accordingly the particle is planar, cylindrical or spherical. For axial dispersion model, initial and boundary conditions were
same as that of [91]. However, for particle phase different types of boundary conditions were taken:

Boundary conditions

\[
\frac{\partial Q}{\partial r} = 0, \quad \text{at } r = 0, \quad (2.13)
\]

\[- \frac{K D_F}{\beta} \frac{\partial Q}{\partial r} = k_f (Q|_{r=R} - C), \quad \text{at } r = R. \quad (2.14)\]

Initial condition

\[Q = C_0, \quad \text{at } T = 0. \quad (2.15)\]

The model was developed in both the axial and radial directions. It was the first model of its kind that considered the effect of axial dispersion and intrafiber diffusion in pulp fibers along with the certain other physical properties of fibers such as radius of fiber pores, fiber porosity, fiber length etc. and the mass transport phenomenon through the fiber pores to the bulk fluid. This model gave an extensive study of the fiber structure, fluid behavior and transport phenomenon.

Garg and Ruthvan [38] gave the solution of Fickian diffusion equation, presented for sorption in a system of spherical particles in which the diffusivity of the sorbate varies with concentration. For the solution, Crank–Nicholson method and explicit finite difference scheme were used:

\[
\frac{\partial C}{\partial T} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( D r^2 \frac{\partial C}{\partial r} \right), \quad (2.16)
\]

where \( C = \) sorbate concentration,

\( T = \) time,
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\( r = \) radial coordinate,

\( D = \) diffusivity.

For a step change in sorbate partial pressure from zero to \( p \) or from \( p \) to zero at time \( T = 0 \), the appropriate initial and boundary conditions, assuming instantaneous equilibration at the crystal surface, were:

\[
C(r, 0) = 0, \quad \text{(adsorption) or } C_0 \text{ (desorption)}, \quad (2.17)
\]

\[
C(r, T) = C_0, \quad \text{(adsorption) or } 0 \text{ (desorption)}, \quad (2.18)
\]

\[
\frac{\partial C}{\partial r}(0, T) = 0. \quad (2.19)
\]

Grahs [40] has developed a model for washing of cellulose fibers. He has divided packed bed into three different zones namely fibrous zone, stagnant zone and zone of flowing liquor. The porosities of different zones were considered separately. Concentration of liquor in stagnant zone was related with amount of solute adsorbed on fiber surface by Langmuir isotherm.

Flowing liquor

\[
\beta \frac{\partial C}{\partial T} + \epsilon_s \frac{\partial C_s}{\partial T} + C_F \frac{\partial N}{\partial T} = \beta D_L \frac{\partial^2 C}{\partial X^2} - \beta U \frac{\partial C}{\partial X}. \quad (2.20)
\]

Stagnant liquor

\[
\epsilon_s \frac{\partial C_s}{\partial T} = k_1 (C - C_s) - C_F \frac{\partial N}{\partial T}. \quad (2.21)
\]
Fibers model

\[ C_F \frac{\partial N}{\partial T} = k_2(C_s - C_s^*). \] (2.22)

Boundary conditions

\[ UC - D_L \frac{\partial C}{\partial X} = UC_s, \text{ at } X = 0, \] (2.23)

\[ \frac{\partial C}{\partial X} = 0, \text{ at } X = L. \] (2.24)

Initial condition

\[ C = C_s = C_s^* = C_0 \text{ and } N = N_0, \text{ at } T = 0. \] (2.25)

Perron and Lebeau [74] have followed one dimensional model to study washing behavior of pulp fibers. Axial dispersion coefficient was totally ignored. The simplified model was solved using Laplace transforms. The results were interpreted using statistical tools. Simulation of an industrial plant using four washers in a row was done using a combination of static and dynamic models.

Bulk fluid model

\[ \beta \frac{\partial C}{\partial T} + \epsilon_s \frac{\partial N}{\partial T} + \beta U \frac{\partial C}{\partial X} = 0. \] (2.26)

Fibers model

\[ \frac{\partial N}{\partial T} = k_f(C - N). \] (2.27)

Boundary condition

\[ C = C_s, \text{ at } X = 0. \] (2.28)
Initial condition

\[ C = N = C_0, \quad \text{for } 0 < T < X/U. \] (2.29)

Raghvan and Ruthven [78] have presented the axial dispersed plug-flow model. Both external and internal diffusional mass transfer resistances are included.

Particle diffusion model

\[ \frac{\partial Q}{\partial T} = D \left( \frac{\partial^2 Q}{\partial r^2} + \frac{2}{r} \frac{\partial Q}{\partial r} \right). \] (2.30)

Boundary conditions

\[ \frac{\partial Q}{\partial r} = 0, \quad \text{at } r = 0, \] (2.31)

\[ D \frac{\partial Q}{\partial r} = k \left( C(X, T) - \frac{Q}{K} \right), \quad \text{at } r = R. \] (2.32)

Initial condition

\[ Q = 0, \quad \text{at } T = 0. \] (2.33)

External fluid model

\[ - D_L \frac{\partial^2 C}{\partial X^2} + U \frac{\partial C}{\partial X} + \frac{\partial C}{\partial T} = \frac{1}{\epsilon} \left[ \frac{3k}{R} \left( C(X, T) - \frac{Q|_{r=R}}{K} \right) \right]. \] (2.34)

Boundary conditions

\[ D_L \frac{\partial C}{\partial X} = -UC, \quad \text{at } X = 0, \] (2.35)

\[ \frac{\partial C}{\partial X} = 0, \quad \text{at } X = L. \] (2.36)

Al-Jabari et al. [5] has followed an axial dispersion model to study filler adsorption on fibers. The concentration of fillers in suspension and concentration of fillers adsorbed on
fiber surface were related via Langmuir adsorption isotherm.

**Axial dispersion model**

\[
\frac{\partial C}{\partial T} = D_L \frac{\partial^2 C}{\partial X^2} - U \frac{\partial C}{\partial X}.
\]  
(2.37)

**Filler adsorption**

\[
\epsilon \frac{\partial Q}{\partial T} + (1 - \epsilon) \rho_f \frac{\partial N}{\partial T} + U \frac{\partial Q}{\partial X} = 0.
\]  
(2.38)

**Initial condition**

\[Q = N = 1, \quad \text{at} \ T = 0.\]  
(2.39)

Kukreja et al. [50] has followed an axial dispersion model of Sherman [91] for linear and finite rate isotherms with Danckwert’s boundary conditions. Models for all zones of a rotary washer were presented.

**Boundary conditions**

\[
UC - D_L \frac{\partial C}{\partial X} = UC_s, \quad \text{at} \ X = 0,
\]  
(2.40)

\[
\frac{\partial C}{\partial X} = 0, \quad \text{at} \ X = L.
\]  
(2.41)

**Initial condition**

\[C = C_0, \quad \text{at} \ T = 0.\]  
(2.42)

The model equations were solved using Laplace transforms. The data of Indian hardwood was used to validate the models. The lab scale pilot plant was used to run the experiments. The values of exit solute concentration, average solute concentration and mean solute concentration were presented at different values of time.
Sun and Levan [96] have considered one–dimensional unsteady diffusion in a spherical particle which is described by the following dimensionless equations:

\[
\frac{\partial X}{\partial T} = \frac{2}{r} \frac{\partial X}{\partial r} + \frac{\partial^2 X}{\partial r^2}.
\]  \hspace{1cm} (2.43)

Boundary conditions

\[
\frac{\partial X}{\partial r} = 0, \quad \text{at } r = 0, \hspace{1cm} (2.44)
\]

\[
X = X_s(T), \quad \text{at } r = 1, \hspace{1cm} (2.45)
\]

where \(X_s(T)\) is variation of the surface concentration with time.

Initial condition

\[
X(r, 0) = 0. \hspace{1cm} (2.46)
\]

They have solved the equations using finite difference method and found that the iso–volumetric discretization performs better than the equal spacing discretization to improve the efficiency of the finite difference method.

Sridhar [94] has studied affinity separation of a packed bed model using non linear adsorption isotherm. Model included mass transfer coefficients, film resistance coefficients and porosities of bed and particle. Solute adsorbed on particle surface and solute inside the particle pores were related using Langmuir kinetics.

Bulk fluid model

\[
\frac{\partial C}{\partial T} + \frac{3(1 - \epsilon)}{\epsilon} \frac{k_f}{\beta R} (C - Q|_{r=R}) = D_L \frac{\partial^2 C}{\partial X^2} - U \frac{\partial C}{\partial X}. \hspace{1cm} (2.47)
\]
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Particle phase model

\[ D_F \left( \frac{\partial^2 Q}{\partial r^2} + \frac{2}{r} \frac{\partial Q}{\partial r} \right) = \frac{\partial Q}{\partial T} + \frac{(1 - \beta)}{\beta} \frac{\partial N}{\partial T}. \]  

(2.48)

Boundary conditions

\[ UC - D_L \frac{\partial C}{\partial X} = C_0, \quad \text{at } X = 0, \]  

(2.49)

\[ \frac{\partial C}{\partial X} = 0, \quad \text{at } X = L, \]  

(2.50)

\[ \frac{\partial Q}{\partial r} = 0, \quad \text{at } r = 0, \]  

(2.51)

\[ - \beta D_F \frac{\partial Q}{\partial r} = k_f (Q|_{r=R} - C), \quad \text{at } r = R. \]  

(2.52)

Initial condition

\[ C = N = 0, \quad \text{at } T = 0. \]  

(2.53)

Potucek [75, 76] has followed an axial dispersion model similar to Brenner [18]. He has studied behavior of softwood pulp fibers based on the results obtained experimentally. The data of washing cell was used to validate the model. The interpretation of numerical and experimental values was made using the statistical tools.

Liao and Shiau [56] have followed an axial dispersion model with linear adsorption isotherm to check the removal of phenol from the solution in the activated carbon and amberlite resins XAD-4 fixed bed adsorbers.

Retardation model

\[ R_d \frac{\partial C}{\partial T} = D_L \frac{\partial^2 C}{\partial X^2} - U \frac{\partial C}{\partial X}. \]  

(2.54)
where \( R_d = 1 + \frac{\rho K(1-\epsilon)}{\epsilon} \).

Boundary conditions

\[
C = C_0, \quad \text{at } X = 0, \quad (2.55)
\]

\[
\frac{\partial C}{\partial X} = 0, \quad \text{at } X = L. \quad (2.56)
\]

Initial condition

\[
C = 0, \quad \text{at } T = 0. \quad (2.57)
\]

Farooq and Karimi [34] have presented a dispersed plug flow model for steady state laminar flow in a tube. The 2-D model was reduced to 1-D model using an iterative techniques and then solved analytically.

\[
\frac{D_\gamma \partial}{r \partial r} \left( r \frac{\partial C}{\partial r} \right) = U(r) \frac{\partial C}{\partial X} - D_\gamma \frac{\partial^2 C}{\partial X^2}. \quad (2.58)
\]

Boundary conditions

\[
C = C_0, \quad \text{at } X = 0, \quad (2.59)
\]

\[
\frac{\partial C}{\partial X} = 0, \quad \text{at } X = L, \quad (2.60)
\]

\[
\frac{\partial C}{\partial r} = 0, \quad \text{at } r = 0, \quad (2.61)
\]

\[
- D_F \frac{\partial C}{\partial r} = k_f C|_{r=R}, \quad \text{at } r = R. \quad (2.62)
\]

Initial condition

\[
C = 0, \quad \text{at } T = 0. \quad (2.63)
\]
Arora et al. [8] have presented models for particle phase and fluid phase. Langmuir adsorption isotherm was used for link concentration of pore liquid with concentration of solute adsorbed on the fibers. Model was verified using industrial data of non wood pulp.

Particle phase model

\[
D_{F} \left( \frac{\partial^2 Q}{\partial r^2} + \frac{1}{r} \frac{\partial Q}{\partial r} \right) - \frac{\partial Q}{\partial T} - C_{F} \frac{(1 - \beta)}{\beta} \frac{\partial N}{\partial T} = 0.
\] (2.64)

Boundary conditions

\[
\frac{\partial Q}{\partial r} = 0, \quad \text{at } r = 0, \quad (2.65)
\]

\[
\frac{k_{f} \beta}{K} (Q - C) = -D_{F} \frac{\partial Q}{\partial r}, \quad \text{at } r = R. \quad (2.66)
\]

Fluid phase model

\[
U \frac{\partial C}{\partial X} + \frac{\partial C}{\partial T} + \frac{2D_{F} (1 - \epsilon)}{R} \frac{\partial Q}{\partial r} \bigg|_{r=R} = D_{L} \frac{\partial^2 C}{\partial X^2}. \quad (2.67)
\]

Boundary conditions

\[
UC - D_{L} \frac{\partial C}{\partial X} = 0, \quad \text{at } X = 0, \quad (2.68)
\]

\[
\frac{\partial C}{\partial X} = 0, \quad \text{at } X = L. \quad (2.69)
\]

Initial condition

\[
C = Q = C_0 \text{ and } N = N_0, \quad \text{at } T = 0. \quad (2.70)
\]
Kumar et al. [51] obtained analytical solution using Laplace transform technique for one-dimensional advection diffusion equation with variable coefficient in a longitudinal finite initially solute free domain. The partial differential equation along with initial condition and boundary condition is written as:

\[
\frac{\partial C}{\partial T} = D_0 f(mT) \frac{\partial^2 C}{\partial X^2} - U_0 \frac{\partial C}{\partial X}. \tag{2.71}
\]

Boundary conditions

\[
C(X, T) = C_0, \quad \text{at } X = 0, \; T > 0, \tag{2.72}
\]

\[
\frac{\partial C(X, T)}{\partial X} = 0, \quad \text{at } X = L, \; T \geq 0. \tag{2.73}
\]

Initial condition

\[
C(X, T) = 0, \quad \text{for } 0 \leq X \leq L, \; T = 0. \tag{2.74}
\]

Kumar et al. [52] have solved first degree, second order, parabolic, partial differential equation of [91] using linear isotherm equation with initial and boundary condition of [74]. For the numerical solution ‘pdepe’ solver of MATLAB software is applied on the axial domain of the system of governing partial differential equations. Same model is also solved by taking non-linear Langmuir type adsorption isotherm to describe the relationship between the concentration of the solute in the liquor and concentration of the solute on the fibers as:
\[ N = \frac{A_0 B_0 C}{1 + B_0 C}, \tag{2.75} \]

where \(A_0\) and \(B_0\) are Langmuir constants.

Dabral et al. [25] have studied temperature variation using the quadratic and cubic B-spline finite element method. Algorithms are also developed to evaluate B-spline basis function as well as to use them for evaluation of temperature distribution.

\[ \frac{\partial C}{\partial T} = \beta \frac{\partial^2 C}{\partial X^2}, \quad (X, T) \in \Omega \times [0, T_1], \tag{2.76} \]

where \(\beta\) is the thermal conductivity, \(\Omega = [0, L]\), and \(T_1\) is final time.

Boundary conditions

\[ C(0, T) = q_1, \quad \text{for } 0 \leq T \leq T_1, \tag{2.77} \]

\[ C(L, t) = q_2, \quad \text{for } 0 \leq T \leq T_1, \tag{2.78} \]

where \(q_1\) and \(q_2\) are the constants.

Initial condition

\[ C(X, 0) = C_0(X), \quad \text{for } 0 \leq X \leq L. \tag{2.79} \]

Goh et al. [39] have solved one–dimensional heat and advection–diffusion equation, given as under. A finite difference scheme has been used for discretized time derivatives and cubic B-spline for interpolating the solutions at each time level. The stability analysis of the scheme is also examined by the Von Neumann approach.
\[
\frac{\partial C}{\partial T} + \beta \frac{\partial C}{\partial X} = \alpha \frac{\partial^2 C}{\partial X^2}, \quad a \leq X \leq b, \quad T \geq 0,
\]

where \(\beta\) is the constant speed of moving fluid and \(\alpha\) is diffusion coefficient in \(X\) direction at time \(T (T \geq 0)\).

Boundary conditions

\[
C(a, T) = g_0(T), \quad (2.81)
\]
\[
C(b, T) = g_1(T), \quad T \in [0, T_1]. \quad (2.82)
\]

Initial condition

\[
C(X, 0) = \phi(X), \quad X \in [a, b]. \quad (2.83)
\]

From the study of above models, it is observed that majority of the investigators have followed an axial dispersion model in one or another form. Kuo [53] was the first to introduce the concept of film resistance in the washing of pulp fibers. Brenner [18], Sherman [91], Kukreja et.al. [50] and Kumar et.al. [52] have presented linear diffusion models for displacement washing of pulp fibers. Goh et.al. [39] and Kumar et.al. [51] have solved one dimensional advection-diffusion equation. Pellett [73], and Liao and Shiau [56] have given a model incorporating the features of both the axial dispersion and intrafiber diffusion. Grahs [40] studied the washing behavior of porous structure of particles by dividing the bed into three zones. Perron and Lebeau [74], and Raghvan and Ruthven [78] solved their 2-D models analytically for linear isotherm. Al-Jabari et.al. [5] studied adsorption of fillers on fibers to strengthen the paper.
Garg and Ruthvan [38], and Sun and Levan [96] have considered diffusion equation in a spherical particle. Sridhar [94] divided the axial domain and solved the model by the moving finite element method. Potucek [75, 76] has followed a linear 1-D axial dispersion model to study the washing behavior of pulp fibers and granular particles. Kil and Bhatia [48] neglected the external mass transfer resistance and assumed that adsorption on the macrospore surface was negligible as compared with the micro particle and used linear isotherm. Saritha and Madras [86] neglected the effect of the axial dispersion coefficient and solved a simple model using linear adsorption isotherm. Farooq and Karimi [34] neglected the intrapore solute concentration and the concentration of solute adsorbed on the fiber surface in their 2-D model. Arora et al. [8] used orthogonal collocation on finite elements using Lagrangian basis to solve the equations for bulk fluid phase and particle phase. Arora and Potucek [10] solved such type of models by neglecting the concentration gradient in the radial direction.

Some other investigators have also contributed to the development of macroscopic and microscopic diffusion models namely, Han [42], Norden et al. [69], Edwards and Rydin [32], Crotogino et al. [24], Wong and Reeve [103], Smith and Duffy [93] and Turner et al. [98]. In the recent literature, similar type of advection-diffusion equations are also solved by ([3], [41], [47], [66], [70], [83]).

2.4 Summary

Since the 1960s, a large number of papers have been published on diffusion problems and these are solved by analytically and numerically as well. One of the today’s most
important challenge for the numerical solution of these type of fluid flow problems is modeling and simulation of flow process. The material involved in these processes is porous. The complete removal of solute requires multistage operations due to slow displacement of solute with wash liquor. But it is simply impossible to have simulation that will yield all the details of washing process in a realistically complicated 3D domain.
Figure 2.1: Mathematical modeling cycle.
Figure 2.2: Mass transfer and mass exchange during washing operation.