Mathematical Modelling of Deep Bed Filtration

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Abstract: Numerous mathematical models have been developed to evaluate both initial and transient stage removal efficiency of deep bed filters. Microscopic models either using trajectory analysis or convective-diffusion equations were used to compute the initial removal efficiency. These models predicted the removal efficiency under favorable filtration conditions quantitatively, but failed to predict the removal efficiency under unfavorable conditions. They underestimated the removal efficiency under unfavorable conditions. Thus, semi-empirical formulations were developed to compute initial removal efficiencies under unfavorable conditions. Also, correction for the adhesion of particles onto filter grains improved the results obtained for removal efficiency from the trajectory analysis. Macroscopic models were used to predict the transient stage removal efficiency of deep bed filters. O'Melia and Ali's model assumed that the particle removal is due to filter grains as well as the particles that are already deposited onto the filter grain. Thus, semi-empirical models were used to predict the ripening of filtration. Several modifications were made to the model developed by O'Melia and Ali to predict the deterioration of particle removal during the transient stages of filtration. Models considering the removal of particles under favorable conditions and the accumulation of charges on the filter grains during the transient stages were also developed. This paper evaluates those models and their applicability under different operating conditions of filtration.

Keywords: *Filtration; Initial stage; Mathematical modelling; Transient stage*

1. INTRODUCTION

Deep bed filtration is an effective process in removing particles of various nature and sizes that are present in water and wastewater. Removal of these particles by deep bed filtration involves complex mechanisms. First, particles in suspension are transported near filter grains by mechanisms such as sedimentation, interception, diffusion, inertia and hydrodynamic effect. However, the effective removal of these particles depends on the attachment mechanism, which depends on the surface forces acting between particles and filter grains when their separation distance becomes in the order of nano-meters. The factors, which affect these forces eventually, affect the performance of deep bed filtration.

Particles in suspension and filter grains will have surface charges. If the charges of particles and filter grains are opposite, then the condition of filtration is said to be favorable as particles will have attractive interaction with filter grains. If the charges of particles and filter grains are of same sign, the condition of filtration is termed as unfavorable as particles will have repulsive interaction with filter grains. Generally, filter media such as sand, glass beads and particles in water or wastewater possess negative surface charge; thus most of the time filtration will occur under unfavorable conditions, if no chemicals are added to alter the conditions. There are two broad stages in deep bed filtration. The first stage is called "initial stage" which is just the starting stage of filtration in which the filter bed is clean and the deposition of particles will occur on the surfaces of filter grains which are clean. Just after the initial stage, the rest of the filtration period is called "transient stage". During the transient stage, deposition of particles will occur on the surfaces of filter grains, which are partially covered by already deposited particles. During the transient stage, the removal of particles can either improve or deteriorate initially, according to the chemical conditions of the suspension and filter medium. Sometimes as soon as the filtration commences there will be an improvement in the removal of particles which is called "ripening stage" followed by "working stage" during which the removal remains almost constant. These two stages together are sometimes termed as transient stage. Then, the removal starts to deteriorate which is called "breakthrough stage" (Jegatheesan, 1999).

2. FILTRATION MECHANISMS

The removal mechanism of particles by a deep bed filter is very complex and depends on the physical and chemical characteristics of the water, particles and the filter medium. The particles to be removed from the suspension are smaller than the pores. It follows that if particles had followed the fluid streamlines, many of them would have never touched a filter grain surface and been removed from the flow. But due to various particle transport mechanisms, particles move across the streamlines and arrive adjacent to a grain surface. When they arrive there, an attachment force has to be present in order for the particles to be retained on the filter grain or on the previously deposited particles. If the deposited particles are entrained again in the flow, a detachment mechanism has to be involved.

2.1. Transport Mechanisms

Particles in a suspension must be transported near filter grains before filter grains capture them by surface forces. Various transport mechanisms are involved in bringing the particles closer to filter grains. These mechanisms are discussed in this section.

Straining: If particles large enough to be strained arrive at the filtration surface, they will form a mat and clog the bed rapidly. Such surface clogging can also take place if the concentration of particles is too high.

Interception: If particles remain in streamlines, which approach the grain surface to within a particle radius, the particle will contact the surface and this is characterized by the ratio (N_R) of the particle diameter to the grain diameter (d_p/d_c).

Inertia: Streamlines approaching a filter grain have to diverge as the flow passes round it. If particles have sufficient inertia, they maintain a trajectory, which causes them to collide with the filter grain and this inertial action is characterized by N_I ($=\rho_p d_p^2 U/18\mu d_c$, where ρ_p is the density of the particle, U is the fluid velocity and μ is the dynamic viscosity of the fluid).

Sedimentation: If the particles are large enough, and have a density significantly greater than that of water, they are subject to a constant velocity relative to the water, in the direction of gravity. The extent to which this will deflect particles from streamlines so that they may contact a grain surface depends on the relative orientation (divergences) of the fluid streamline velocity vector and the gravitational velocity vector. The effect of sedimentation may be characterized by $N_G = (\rho_p-\rho)d_p^2 g/18\mu U$, which may be recognized as the ratio of Stoke's velocity for the particle to the fluid approach velocity (ρ is the density of fluid).

Diffusion: Brownian motion is observed to impart a random movement to very small particles in water, due to the thermal energy of the water molecules. For particles less than 1 μm, the movement becomes increasingly significant with decreasing sizes. This mechanism is expressed in terms of the Peclet number, $N_{Pe} = d_c\ U/D$, being the ratio of movement due to Brownian action, i.e. advective motion of the fluid (D is the Stokes-Einstein diffusion coefficient).

Hydrodynamic action: The flow in the filter pores is laminar, with a velocity gradient. Therefore there exists a shear field. In a uniform shear field, a spherical particle would experience rotation with a consequent accompanying spherical flow field. This would cause the particle to migrate across the shear field, in a manner analogous to, but not identical with, the swerving path of a spinning ball in flight. Non-uniform shear field, shape of particles and deformability of particles will all affect the trajectory of the particle. The net result is that particles will exhibit an apparently random, drifting motion across the streamlines, which may cause them to collide with grain surfaces. This is characterized the mechanism by simple Reynolds Number ($Re = d_c U/\nu$) for the filter bed.

Orthokinetic flocculation: Although scarcely a mechanism for transporting particles to grain surfaces, it has been suggested by Camp that Orthokinetic (velocity gradient) flocculation in the filter pores could aggregate particles, thus enhancing their probability of removal (Ives, 1970).

It is unlikely that any of these mechanisms acts uniquely. Particles in the flowing suspension will be subject to all of them in varying degrees; their relative importance will depend on the fluid flow conditions, the geometry of the filter pores and the nature (size, shape, density) of the particles. Experiments are difficult to perform which isolate the action of each mechanism. Yao (Jegatheesan, 1999) has shown that there exist a minimum in filter efficiency at about 1 μm for spherical plastic particles where the particles of this size were too large for diffusion and too small for interception and sedimentation to be significant.

2.2. Attachment Mechanisms

In deep bed filters, various surface forces affect attachment of the particles onto the collector (filter grains). The forces involved in attachment can be divided into two groups. One group consists of the London van der Waals attraction force (F_V) and the electric double-layer force (F_e) (either attractive or repulsive). These forces are called long-range forces as they influence transport and attachment even when a particle is separated from a collector by 100 nm. The second group of forces is Born repulsion force (F_B) and structural or hydration force (F_h). They are termed as short range forces due to their influence on particles is dominant only if the particles are up to 5 nm away from collectors.

2.3. Detachment Mechanisms

There is evidence that an increase of the flow rate through a filter will detach particles causing a more turbid filtrate. The intensity of this effect depends not only on the magnitude of the increase of the flow rate, but also on the rate of change of the flow rate. The effect is diminished if polyelectrolytes are added to the suspension to be filtered. If the flow rate is maintained constant, which is the normal mode of operation of rapid filters, opinions differ on whether detachment takes place. The principal proponent of detachment is Mints (Ives, 1970) whom considered that the structure of accumulated deposits in a filter medium is not equally strong. Under the action of hydrodynamic forces caused by the flow of water through the media with increasing headloss, this structure is partially destroyed. A certain portion of previously adhered particles, less strongly linked to the others, is detached from the grains as long as new particles are being supplied.

Another group of researchers opposed this detachment mechanism. They stated that, as the interstitial velocity increases and as the surface available in the filter pores and the amount divergence and convergence of flow diminish because of the deposits accumulating in the pores, there is a reduction in the probability of particles being brought to a surface for adherence. However, at present, both groups agree the concept of detachment.

3. MATHEMATICAL FORMULATIONS FOR FILTER EFFICIENCY

Many researchers have discussed on the factors responsible for removal of suspended solids within the filter. Their research could be broadly classified into two major groups namely macroscopic and microscopic approaches. In deep bed filtration, mathematical models based on the macroscopic approach deals with cumulative collection of deposits whereas the microscopic approach considers the individual particle size and the number of particles.

3.1. Microscopic Approach

In microscopic approach the filter bed is modelled as an assemblage of single or unit collectors, which have a particular geometry, and around or through which fluid flows. The fluid flow can be analytically described.

Porous Media Models: A variety of porous media models have been proposed to study the various physical or chemical phenomena, such as fluid flow, heat and mass transfer, chemical reaction, that take place in granular media. In principle, any porous media model can be used in filtration studies. Following are the most commonly used models: (i) Capillary model, (ii) Spherical models - Isolated sphere model, Happel's model, Kuwabara's model, Brinkman's model (iii) Constricted tube model (Tien, 1989).

Computation of the Initial Collection Efficiency, η_o: The performance of a filter is expressed in terms of single collector efficiency (η_o) which is defined as the ratio between the Quantity of particles in contact with the collector in a unit time and the Flow rate of particles. Here a single filter grain is termed as collector. Once the value of efficiency of single collector is known, one can calculate the efficiency of the entire bed by using the following equation:

$$[C/C_o] = \exp[(-3/4) \times (1-f_o) \times \alpha\eta_o \times L/a_c] \qquad (1)$$

where C and C_o are the effluent and influent concentrations respectively and α is defined as the ratio between the number of contacts which succeeded in producing adhesion and the number of collisions which occur between suspended particles and the filter grain. Thus α reflects the chemistry of solution, suspended particles and filter grain. Ideally, α is equal to unity in a completely destabilized system. Therefore, the determination of the initial collection efficiency is important in predicting the performance of a clean bed filter.

There are two theoretical approaches for calculating the particle deposition rate onto model collectors from flowing suspensions, namely Lagrangian and Eulerian. Lagrangian methods describe the trajectory of the particle that is governed by Newton's second law as the particle approaches the collector surface, while Eulerian methods describe the particle concentration in time and space. The effect of diffusion cannot be directly included in the trajectory calculations as the trajectory calculations are deterministic. Thus, the trajectory analysis is limited to non-Brownian particles.In the Eulerian approach, the difficulty of accounting for Brownian effects is eliminated.

Eulerian Method - Convective Diffusion Equation: The general convective diffusion equation describing the temporal and spatial variation of particle concentration can be given as:

$$\frac{\partial C}{\partial t} + \nabla.(\vec{u}C) = \nabla.(D.\nabla C) - \nabla.\left(\frac{\vec{D}.\vec{F}}{kT}C\right) \qquad (2)$$

where, C is the particle concentration, t is the time, $\vec{u}$ is the particle velocity vector, $\vec{D}$ is the particle diffusion tensor, $\vec{F}$ is the external force vector, k is the Boltzmann constant and T is the absolute temperature of the suspension. Thus, the first and second terms on the left hand side of eq. 2, denote the temporal variation of the concentration at any point and the transport of particles due to advection at that point respectively. Similarly, the first and second terms on the right hand side describe the transport of particle due to diffusion and external forces respectively.

The convective diffusion equation can be solved analytically, if only a single transport mechanism is considered to be in operation. Levich (1962) developed an analytical solution for the transport rate towards the collector when diffusion was considered as single transport mechanism. This transport rate will be equal to the deposition rate (single collector efficiency due to diffusion = $\eta_D = 4.0\ N_{Pe}^{-2/3}$) when there are no repulsive force between the particle and the collector surface. Similar analytical expressions for the efficiencies due to sedimentation ($\eta_G = N_G$) and interception ($\eta_I = 1.5\ N_R^2$) are combined to obtain the single collector efficiency, η_o:

$$\eta_o = \eta_D + \eta_I + \eta_G \quad (3)$$

Above expressions were obtained using the Stoke's equation for the velocity distribution in the packed bed. If sphere-in-cell model developed is used to describe the velocity terms, η_D is considered to be $4.0\ A_s^{1/3}\ N_{Pe}^{-2/3}$, where A_s is the porosity term that is defined as, $A_s = 2(1-p^5)/w$; $p = (1-f)^{1/3}$; $w = 2 - 3p + 3p^5 - 2p^6$, where f is the porosity of the filter bed. Levich's model was formulated for favorable chemical conditions. Spielman and Friedlander (Elimelech, 1994) developed an interaction force boundary layer (IFBL) model in which they considered two distinct regions near the surface; an inner region (the IFBL) and an outer region (the diffusion boundary layer). Convection influences the outer region and the colloidal interactions are confined to the inner layer. The solutions of the convective diffusion equation (i) for the outer layer in the absence of surface forces and (ii) for the inner region without the convection are matched. The analytical solution obtained by them for Brownian particles under repulsive EDL interaction is given elsewhere (Jegatheesan, 1999).

In order to calculate the collision efficiency, α (which is the ratio of the collector efficiency in the presence of the repulsive EDL forces to that of the collector efficiency under favorable conditions = η/η_o), η_o of the Brownian particle was taken as $4.0\ A_s^{1/3}\ N_{Pe}^{-2/3}$.

Thus the models explained above were solutions for the convective diffusion equation under certain physical and chemical conditions. A rigorous numerical solution for the convective diffusion equation to employ under any circumstance (i.e. repulsive as well as attractive EDL interaction), was put forward by Elimelech (1994). From the numerical solution, the effects of various parameters, such as ionic strength, particle size, surface potentials of particles and collectors, Hamaker constant of the interacting media, and the double-layer interaction mode, on initial collection efficiency can be predicted.

Lagrangian Method - Trajectory Analysis: In the trajectory analysis, it is assumed that the deposition occurs once a particle comes into contact with the collector. The forces generally taken into account are gravitational, hydrodynamic and surface forces. The phenomenon of interception of particles by the collector is incorporated in the boundary conditions.

3.2. Comparisons Between Experiments and Theoretical Predictions

IFBL results: Experimentally calculated collision efficiency, α (Elimelech, 1994) under repulsive double layer interactions yielded different results from the theoretical predictions. From the experiments, it was found that α and critical deposition concentrations are independent of particle size. The reasons for this discrepancy is due to: (i) the degree of sensitivity of α to the ionic strength of the solution; (ii) the electrokinetic potentials of particles and collectors are less than predicted; (iii) surface charge heterogeneity and surface roughness of particles and collectors; (iv) deposition in secondary minima; and (v) necessity to consider the interfacial dynamics of double-layer interaction.

Numerical Solution by Elimelech (1994): The numerical solution can be applied both for attractive and repulsive double-layer interaction. Theoretical predictions were found to match with experimental results under attractive double-layer interaction.

Trajectory Analysis: Agreement between experiments and predictions is limited to those occasions when conditions, that is, surface interactions are favorable. The conclusions based on trajectory analysis, in the case of unfavorable surface interaction, are at total variance with experiments. Even when surface interaction is favorable, systematic errors were observed when predicting initial filter coefficient for large particle sizes (Tien, 1989). The data reported by Gimbel and Sontheimer (Tien, 1989) cover a much greater particle size range than other similar studies. They found that the filter coefficient is relatively independent of particle size and that predictions based on Happel's model tend to overestimate at high values of d_p values and underestimate at lower d_p values. One may adjust for this discrepancy, however, by considering particle adhesion. In spite of severe limitations, trajectory analysis has been found as useful to explain the initial removal efficiency of a filter.

3.3. Improvements to the Models

Elimelech (1992): According to theoretical prediction, particle size has a marked effect on the collision efficiencies in the region of unfavorable deposition. It predicts that at given chemical conditions, the collision efficiencies decrease as the particle size of the suspension increases. The lack of dependence of experimental collision efficiencies on particle size leads to a formulation of an empirical relationship (Elimelech, 1992):

$$\alpha = g(\Theta, \kappa, A) \quad (4)$$

where $\Theta = \varepsilon_o \varepsilon_r \psi_1 \psi_2$ The dimensional analysis yields the following linearized form :

$$\log \alpha = \log B + n \log (\kappa A / \Theta) \quad (5)$$

where B and n are constants to be determined from experimental values of $(\kappa H/\Theta)$ and α.

Bai and Tien (1996): Bai and Tien developed a correlation for the initial filter coefficient under unfavorable surface interactions. By applying the Buckingham-π theory, α is shown to be a function of 11 dimensionless parameters. Further, by conducting partial regression analysis to available experimental data, only 4 of the 11 dimensionless parameters were found to exert strong influence on α.

$$\alpha = 10^{-2.9949} (N_{LO})^{0.8495} (N_{E1})^{-0.2676} (N_{E2})^{3.8328} (N_{DL})^{1.6776} \quad (6)$$

where, N_{LO} is the London number, N_{E1} first electrokinetic parameter, N_{E2} second electrokinetic parameter and N_{DL} is the double layer force parameter. The dimensionless parameter $(\kappa A/\Theta)$ used by Elimelech (1992) is a combination of the four parameters N_{LO}, N_{E1}, N_{E2} and N_{DL}.

Improvement through the introduction of particle adhesion model: Vaidyanathan (Tien, 1989) proposed two methods based on particle adhesion to improve the theoretical prediction on initial filter coefficient. Details of which can be seen elsewhere (Jegatheesan, 1999). The experimental values obtained by Gimbel and Sontheimer for the λ_o of larger particles deviated significantly from the corresponding λ_o values obtained by trajectory analysis. However, by correcting for attachment efficiency, better agreement was obtained between theoretical and experimental λ_o values.

3.4. Macroscopic Approach

In the macroscopic approach, the physical and chemical characteristics of suspension and the flow field of granular bed are not explicitly accounted for. The effects of such parameters as particles size and particle and solution chemistry are implicitly included in the value of the filter coefficient, λ. The value of λ cannot be predicted beforehand but is determined from the experimental results of the specific system.

Iwasaki (1937) made the initial attempt at a mathematical description of granular media filtration. Iwasaki (1937) proposed an equation based on first order kinetics, which was then verified experimentally by Ison and Ives (1969).

$$-\partial C/\partial L = \lambda C \quad (7)$$

where, C = concentration of particulate matter at a given time and depth, L = filter depth, λ = filter coefficient. The general form of material balance of particles in an element of filter depth (ΔL) and a cross-sectional area of (A) at a time t can be written as:

$$\partial[A(\sigma+fC)]/\partial t + \partial(AUC - AD\, \partial C/\partial L)/\partial L = 0 \quad (8)$$

where $A\sigma$ is the volume of particles retained in a unit depth filter, AfC is the volume of particles in motion entrained by liquid in a unit depth of filter, AUC is the particle flow entrained by the fluid, $-AD(\partial C/\partial L)$ is the diffusional flux of particles, f is the porosity of clogged bed ($f=f_o - \beta\sigma$), f_o is the clean bed porosity, β is the inverse of compactness (actual volume of deposit/ compacted volume of deposit), and σ is the specific deposit. Assuming, the velocity of suspension is constant throughout the filter run, the diffusion of particles is negligible for particles of size greater than 1 μm, the concentration of suspension is as low as 0.1% in water filtration, which makes the term $\beta\sigma$ negligible compared to f_o (i.e $f=f_o$) and the term fC is negligible compared to σ, eq.8 can be simplified as:

$$-\partial C/\partial L = 1/U\, \partial\sigma/\partial t \quad (9)$$

Combining eq.7 and 9,

$$\partial\sigma/\partial t = \lambda UC \quad (10)$$

The governing parameters of the macroscopic model λ and σ (appearing in the above equation) are implicit functions of physical and chemical characteristics of suspension and filter medium in addition to filtration velocity. They vary during the process of filtration with time and filter depth. In order to predict the concentration profile, one should know the value of λ. The most general equation is the one proposed by Ives (1969) who has taken into account the variations of specific surface of medium by the accumulation of deposit, porosity and interstitial velocity by the retention of particles. It is interesting to note that the coefficients appearing in these equations are functions of suspension, filter medium characteristics and operating parameters. Therefore, once these coefficients are calculated from pilot-scale or laboratory-scale experiments with the given suspension and medium, one can simulate the concentration profile for the same suspension for different operating parameters using eq.7 and 9 and the relationship between λ and σ.

Macroscopic approach in general does not explicitly describe the physical and chemical characteristics of filter medium, suspension and flocculant used. They are included only as implicit functions of λ and σ.

3.5. Models for Transient Stage Filter Efficiency

Particle removal in deep bed filtration is physico-chemical in nature and depends on the physical and chemical characteristics of particles, filter grain, water and chemicals used. A number of mathematical models have been developed to calculate particle capture in the filter. Four such models are described in this section, which predict the removal efficiency during transient condition of a filter:

Model 1: Based on the assumption of detachment of retained particles Model 2: Based on the analogy of filtration and adsorption; Model 3: Based on blocking; Model 4: Based on the effect of the change in the surface charge of filter grains.

Limitations of the models for transient stage filter efficiency: It is noted by Vigneswaran and Chang (Jegatheesan, 1999) that the model based on the detachment mechanism (Model-1) can simulate the filter performance satisfactorily and easily at all filtration velocities whereas the model based on the analogy of adsorption (Model-2) can simulate satisfactorily the filter performance at low filtration velocity. Inclusion of factors related to the attraction and electric double-layer interaction forces in the transient state modeling in an explicit manner is required.

In the third model (Johnson and Elimelech, 1995), parameter optimization and curve fittings are eliminated as the model can be obtained using the known parameters together with theoretical coefficients. Excellent agreement between the theoretical curves (based on the random sequential adsorption (RSA) mechanism) and experimentation was observed for the wide range of ionic strengths. Thus RSA mechanism can be used to predict the transient stage, irreversible monolyer, deposition of colloids. However, this model cannot be applied for unfavorable surface conditions as the deposition of colloids will be reversible due to repulsive double-layer interaction between the surfaces of colloids and filter grains.

The fourth model (Tien, 1989) is useful in predicting the charge accumulation on the filter grain surface due to the deposition of particles. However, the model is valid in predicting the changes in the filter media structure only at lower interception number (N_R = particle diameter/filter grain diameter) and/or for small amount of deposition of particles (Tien, 1989). Even then, the model predictions did not agree with the results of some of the experiments conducted under the above mentioned conditions (Tien, 1989).

4. CONCLUSIONS

Numerous models to predict the removal efficiency in deep bed filtration at initial and transient stages have been examined in this paper. However, efforts are still under way to develop a model that can describe the entire filter cycle. The long history in the deep bed filtration research would definitely make this an achievable task in the future.

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